THE MATHEMATICAL THEORY
OF SYMMETRY IN SOLIDS

Representation theory
for point groups and space groups

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Preface

As the sub-title suggests, this book is devoted to the theory of the deduction of the irreducible representations of point groups and space groups and to their tabulation, together with some discussion of the determination of symmetry-adapted functions that belong to these representations. Some consideration is also given to the co-representations of magnetic point groups and space groups. Most of the theory of the determination of space-group representations is, of course, available already in the literature, but it is very scattered and different authors have used various sets of notation. Two sets of tables of space-group representations have been published for some time (Faddeyev 1964, Kovalev 1965), but neither included any very comprehensive account either of the theory or of the properties of these representations; at a very late stage in the preparation of this manuscript the work of Miller and Love (1967) was published and at the proof stage the work of Zak, Casher, Glück, and Gur (1969) also became available. We have made use of all these works in checking many of our tables.

Complete tables are given of the single-valued and double-valued representations of the group of **k** at each point of symmetry and along each line of symmetry in the Brillouin zone of each of the 230 space groups. These tables include all the relevant abstract finite groups (of order ≤ 192) and we identify the group of each wave vector **k** in terms of the appropriate abstract group. In these tables both the character tables and the matrix representatives are given. Several of the tables have been derived or checked by computer, specifically Tables 2.6, 5.1, 5.7, and 6.8, but we shall not give any description of the computing techniques involved and refer the reader, for example, to the review article on computers and group theory by Cannon (1969). The compatibility of Table 6.13 with Table 5.7 has also been checked, by hand; see the footnote on p. 468. Comparison with existing sets of tables for some individual space groups and with the tables of Faddeyev, Kovalev, Miller and Love, and Zak, Casher, Glück, and Gur has been made, but a completely exhaustive comparison with all the existing work has proved impossible because of the many different notations and conventions that have been used by different authors. It would be very remarkable indeed if all the entries in these tables were correct, and we should be extremely grateful to receive details of any errors that readers may find. An arrangement has been made with the Institute of Physics for the publication of such errors that come to our notice in the form of Letters to the Editor of *Journal of Physics C: Solid State Physics*.

We have included as much as seemed to be necessary of the description of the mathematical crystallography of Bravais lattices, point groups, and space groups, but the reader may find it profitable on occasions to refer either to one of the various textbooks on crystallography or to the *International tables for X-ray crystallography* (Henry and Lonsdale 1965). In Chapter 3 we give a partially complete account of representation theory for space groups. The complete theory is presented in Chapter

4 in which we treat the theory in a general notation so that we cover not only the theory of space groups but also obtain a theory that is useful in other applications outside the theory of solids. It is hoped, therefore, that parts of Chapter 4 will be of use, as a preliminary study in the theory of induced and subduced representations, to workers in a variety of fields and not just to solid-state physicists. We have assumed that the reader has a basic working knowledge of the theory of groups and of group representations; however, we have summarized the relevant parts of this theory in sections 1.2 and 1.3.

Some omissions have necessarily been made. We have omitted any discussion of the symmetry properties of tensors in crystals partly because it makes little use of representation theory and partly because the subject of the symmetry properties of tensors is already well-documented both for non-magnetic crystals (Nye 1957) and for magnetic crystals (Birss 1964). Although we have given some careful consideration in Chapter 7 to the theory of the corepresentations of magnetic space groups and have given some examples, it has not been practicable, in the space available, to include tables of the irreducible corepresentations of all the 1191 black and white magnetic space groups; these are all tabulated by Miller and Love (1967). We should have liked to have included some detailed discussion of the fields in which the theory and the tables that we have given can be applied. However, neither space nor time was available to do this properly, since this would probably need a second large volume; therefore, at appropriate points in the text we have simply indicated possible physical applications and given references to suitable treatises or review articles. Finally, we have omitted any discussion of the non-crystallographic point groups on the grounds that they do not properly belong in a book that is concerned primarily with solids rather than with molecules.

We are particularly grateful to Dr. S. L. Altmann, who provided much of the original stimulus for the writing of this book and who has watched its progress with considerable interest, and to the various people with whom we have had helpful discussions or correspondence about either text or references at various stages; Dr. J. S. Rousseau and Dr. N. B. Backhouse for a careful reading of various chapters which led to the removal of a number of errors; Dr. B. L. Davies, for extending the tables of cubic lattice harmonics in Chapter 2 from an accuracy of 8 to 11 decimal places and for some general assistance with parts of Chapter 7 and some of the Russian references; Dr. R. J. Elliott; Dr. G. Harbeke; Dr. K. L. Jüngst, who carried out an independent check on the tables of lattice harmonics in Chapter 2 and subsequently provided a few corrections; Dr. D. Litvin; Prof. R. Loudon; Dr. W. Marzec, for supplying a list of corrections to the tables of Kovalev (1965); Dr. K Olbrychski; Dr. M. Schulz; Mr. J. Staněk, for some help with the indexing of chapter 7; Mr. D. E. Wallis, for writing computer programs to check Table 5.1; Mr. R. H. Whittaker and Prof. J. Zak. One of us (A.P.C.) would like to record the fact that most of his contributions to the writing of this book were made during his two previous appointments, in

the Physics Departments of the University of Singapore and the University of Essex, and he is grateful to his former colleagues for their interest and encouragement during those times. We are grateful to the various authors, editors, and publishers who have granted permission to reproduce copyright figures and tables, the sources of which are indicated appropriately *in situ*. Finally, we are also grateful to the staff of the Clarendon Press for the care with which the production has been handled.

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Symmetry and the solid state

1.1. Introduction

THE history of man's interest in symmetry goes back many centuries (Belov 1956*b*, Coxeter and Moser 1965, Steno 1669), but its study on a modern scientific basis can be considered to have been started by the Abbé Haüy. Haüy studied the behaviour of a specimen of calcite when it was cleaved and, by breaking it into smaller and smaller pieces and studying the angles between the faces of the fragments, he convinced himself that the crystal was made up by the repetition of a large number of identical units. Haüy (1815*a–d*) studied many other crystals as well and summarized his conclusions in his so-called *Loi de symmétrie*. The study of symmetry developed through the nineteenth century with the formulation of ideas about point groups, Bravais lattices, and space groups.

A *point group* is a set of symmetry operations acting at a point and obeying the requirements that they should form a group in the mathematical sense; the crystallographic point groups satisfy the extra requirement that they must be compatible with a space lattice. Only a finite number of different combinations of symmetry operations are observed to occur in real crystals. The derivation of these 32 point groups was published by Hessel (1830) but his work was neglected for over 30 years until they were derived again by Gadolin (1869). Since then the point groups have been studied extensively, both in their original crystallographic context and, more recently, in the context of group-theoretical studies of the physics and chemistry of molecules and solids. There are useful crystallographic texts, for example, by Buerger (1956) and Phillips (1963*a*). General discussions of the theory associated with the applications of the group-theoretical studies of the point groups are given by many authors (for example; Bhagavantam and Vankataryudu 1962, Cracknell 1968*b*, Hamermesh 1962, Heine 1960, Tinkham 1964).

We can also consider another collection of groups, this time by considering translational symmetry operations. If we were to look at the internal structure of a crystal we would find that it is made up of a large number of atoms or molecules regularly arranged; it would be possible to find a set of points within the crystal which are similar. That is, the crystal looks exactly the same if viewed from any one of these points as it does if it is viewed from any other of them. If we consider such a set of identical points they make up what the mathematicians call a *lattice*. It is possible to show that there is only a small number of essentially different ways of arranging a set of identical points so that the environment of each one is the same. This was done by Bravais (1850) who showed that in a three-dimensional space there are only

14 different lattices possible; consequently these are now known as *Bravais lattices*, even though Frankenheim had deduced, incorrectly, 15 such lattices somewhat earlier.

A point group is concerned with the symmetry of a finite object and for natural crystals there are only 32 different point groups; a Bravais lattice is concerned with the arrangement in space of a collection of mathematical points. To study fully the internal structure of a crystal, that is, the exact detailed arrangement of the atoms within the unit cell of a crystal, one needs a further development of symmetry studies known as a *space group*. A space group takes into consideration the symmetry of an arrangement of a set of identical objects, each of which is now not a point but is a finite object or a collection of atoms having some symmetry of its own. The actual operations present in a space group may be operations of the type which are present in point groups, namely pure rotations, reflections, the inversion operation, and roto-inversion or roto-reflection operations. But other operations are possible as well in a space group: they are screw rotation—and glide reflection operations—of symmetry. These are symmetry operations in which either a rotation axis or an ordinary reflection plane has a bodily movement of the crystal combined with it. In the descriptions of the derivation of the 230 space groups it is usually indicated that we owe them to Fedorov and Schönflies and sometimes the name of Barlow is added. A review of the history of the derivation of the space groups, together with a list of the publications of Barlow, Fedorov, and Schönflies, is given in an article by Burckhardt (1967). The derivation of the space groups has its origins in the works of Jordan (1868, 1869) and of Sohncke (1879). Sohncke had derived those space groups, of which there are 65, that contain only proper rotations and he noted that Jordan had previously derived them mathematically but had not translated his results into the more graphic terms of geometry. Schönflies re-derived these 65 space groups and extended the theory to include the space groups containing reflection planes of symmetry (Schönflies, 1887a, b, 1889, 1891). Similar results were derived by Fedorov (1885, 1891a) but his work was written in Russian and has not become so well known in western Europe; an account of the life and work of E. S. Fedorov and a list of his publications is given (in Russian) in the book by Shafranovskii (1963). It is evident that these two scientists began their works independently, one (Fedorov) as the director of a mine in the Urals and the other (Schönflies) at the suggestion of F. Klein at Göttingen, but in the course of time they heard of each other's work and compared their results. Barlow (1883) was first concerned with spherical packings and then starting with Sohncke's 65 groups he, too, obtained the remaining space groups by including reflection operations of symmetry (Barlow 1894). Burckhardt (1967) concludes that although Schönflies was not actually the first to establish the existence of the 230 space groups his writings have been the means of making their enumeration and identification generally known to the scientific world. His work, which is but little later than that of Fedorov and is quite independent, culminates in the book

Krystallsysteme und Krystallstructur (Schönflies 1891). A letter from Schönflies to Fedorov, quoted by Burckhardt (1967), reads 'I express my great joy about the agreement with your own views; I am particularly pleased, because I am no longer alone with my theory; it will still take great efforts before we shall succeed in winning over the crystallographers. *I concede you the priority with pleasure*, it is of no primary importance to me.' A convenient detailed list of the space groups in modern notation can be found in Volume 1 of the *International tables for X-ray crystallography* (Henry and Lonsdale 1965). At the present time there are about 9000 compounds whose space groups have been identified (for recent lists see Donnay, Donnay, Cox, Kennard, and King (1963), Nowacki, Edenharter, and Matsumoto (1967), and Wyckoff (1963, 1964, 1965, 1966, 1968)). The discovery of the two-dimensional space groups, which are also listed in detail in Volume 1 of the *International tables for X-ray crystallography*, is lost in the mists of antiquity because they arose in practice, in many different civilizations, in the designs of wallpapers or tiled floors (see, for example, Coxeter and Moser (1965), p. 33).

Although studies of a vast number of crystal structures had been undertaken by X-ray methods and these crystals had been assigned to the appropriate space groups, the study of the theory of symmetry seemed not to advance very much, after the derivation of the 230 space groups in about 1890, until Shubnikov in 1951 published a book called *Symmetry and anti-symmetry of finite figures* (in Russian, though this work is now translated into English, together with a list of many references to other works of Shubnikov (Shubnikov and Belov 1964)). A review of the developments in the theory of symmetry over the last 50 years is given by Koptsik (1967*a*) and a brief biography of A. V. Shubnikov is given at the beginning of volume 2 of *Kristallografiya* (*Soviet Phys. Crystallogr.* (English transl.) (1957)). The new developments were connected with introducing an operation of *anti-symmetry*. The classical theory of symmetry, point groups, Bravais lattices, and space groups, was essentially a 3-dimensional study, that is, a point P would be specified by the vector $\mathbf{r}\{ = (x, y, z)\}$, and we would consider the effect of symmetry operations on this point. Shubnikov's basic idea was to say that in addition to the ordinary coordinates x, y, and z of a point we now also give each point a fourth coordinate, s, which can only take one of two possible values. The coordinate s can be the spin of a particle and the two allowed values will then correspond to spin up and spin down. Or, in purely abstract terms, they may be two colours such as black and white. If we include the coordinate s and if the values of s for the various atoms are randomly specified then the symmetry of the lattice has been completely destroyed. But if the spins are all parallel to a particular direction or if they are arranged in some regular fashion it is possible for some fraction of the symmetry to survive. If we introduce a new operation, which we may call the *operation of anti-symmetry*, $\mathscr{R}$, and consider this in conjunction with all the ordinary point-group and space-group operations it is possible to obtain a whole collection of new point groups and space groups which are called *black and white groups*, or

magnetic groups, or *Shubnikov groups*. The idea of black and white groups was actually introduced long before Shubnikov's work, by Heesch (1929*a*, *b*, 1930*a*, *b*) and also discussed by Woods (1935*a–c*), but at that time there seemed to be no very great use for these groups in the description of physical systems. It was only with the introduction of the use of neutron diffraction techniques that it became apparent that these groups could be used in the description of magnetically ordered structures. If we think of s as being the two allowed values of a magnet's direction, parallel and anti-parallel to a particular direction, then $\mathcal{R}$ is the operation that reverses a magnetic moment. $\mathcal{R}$ can then be thought of as being the operation of *time-inversion*.

The theory of finite groups dates from the time of Cauchy[‡] who was responsible for noticing that a number of apparently disconnected facts could be explained simultaneously by introducing the concept of a group. Galois[§] added to the theory a number of new concepts, including that of an invariant subgroup, and part of his work on the theory of equations was a first and most startling example of the power of group theory in its applications. However, it is to Serret (1866) that we owe the first connected account of group theory. Since then there has been an increasing flow of literature on the subject and today abstract group theory still flourishes as a major topic for research. Furthermore, the variety of applications of finite groups in a host of mathematical situations as diverse as the theory of permutations, the study of symmetry, and the theories of algebraic and differential equations, to mention just a few, means that a study of groups is essential for those engaged in many disciplines requiring mathematical techniques. The natural sciences are riddled with examples of problems requiring a knowledge of group theory and it is a safe assumption that the biological sciences and perhaps even the social sciences, as they become increasingly mathematical, will produce further interesting applications.

In a mathematical theory it is often possible to pick out a number of famous scholars who have been responsible for the major advances. Group theory is no exception. The only fear we have in mentioning certain names is that those of many others who have made great advances are likely to be omitted. However, it is surely no injustice to single out the names of Sylow, Frobenius, Burnside, Schur, Miller, and Mackey (apologizing immediately to Noether, Brauer, Ito, and many others who have made great contributions to the theory of abstract groups but whose work is not so directly related to the applications in this book).

Sylow (1872) made considerable progress in describing the structure of a finite group particularly in relation to its number of elements when this number is factorized as a product of primes. Frobenius (1896*a*, *b*, 1898) originated and was largely responsible for the theory of group representations and group characters, though Burnside (1903, 1911) made such significant simplifications and was responsible for so many original results that he also must be thought of as a group theoretician of great influence.

As a worker with a prodiguous output (of approximately 800 papers between 1894 and 1946) Miller (1894, 1946) devoted considerable attention to the investigation of the structures and properties of various groups of finite order. He was responsible for determining the numbers of finite groups of various specific orders and studying the interrelationships between the structures of these groups, as exemplified by their generating relations.

The study of relations between representations of a group and those of an invariant subgroup leads inevitably to projective representations. Schur was the first to notice this and in an astounding sequence of definitive papers (1904, 1907, 1911) he not only laid the foundations of the general theory of projective representations but established most of the results that are regarded as being of particular significance. Again it was Frobenius (1898) who was responsible for the first construction of what is now called an induced representation. However, this particular notion, so important to applications in physics, was not developed significantly until after 1950 when Mackey in a series of papers (1951, 1952, 1953a, b, 1958) made extremely important advances that already find considerable application not only in the theory of space groups but throughout the whole realm of theoretical physics (see also Mackey (1968)).

We have described the importance of point groups, Bravais lattices, and space groups in specifying both the macroscopic symmetry of a crystal, as determined by goniometry, and the symmetry of the internal structure of a crystal, as determined by X-ray diffraction or neutron diffraction experiments. In classical physics there are some applications of group theory, such as, for instance, the investigation of the normal modes of vibration of a molecule or solid (Wigner 1930) or the determination, for a crystal belonging to a given point group, of relationships that may exist between the various components of a tensor describing some macroscopic property (see, for example, Nye (1957)). However, it was with the advent of quantum mechanics that all the powerful mathematics of group theory and representation theory really became most useful in helping to understand physical systems. Much of the pioneer work on the application of group theory in quantum mechanics was done by Weyl, Wigner, and von Neumann (see Weyl (1931), the translation of the classic book by Wigner (1959) and the collected works of von Neumann (1961, 1963)). In studying a crystal at the microscopic level one has to remember that each of the individual particles of which the crystal is composed obeys quantum mechanics rather than classical mechanics and therefore has to be described by an appropriate wave function ψ. The key to the application of group theory to quantum mechanics lies in the result that is expounded in Chapter 11 of Wigner's classic book (English translation, Wigner (1959)). If a quantum-mechanical system is described by the appropriate Schrödinger wave equation Wigner's theorem can be summarized as follows: '*the representation of the group of the Schrödinger equation which belongs to a particular eigenvalue is uniquely determined up to a similarity transformation.*' Apart from accidental degeneracies this representation will be irreducible. The irreducible representations are

therefore important because they can be used to label unambiguously the energy
levels of a quantum-mechanical system. The irreducible representations of the crystal-
lographic point groups and double point groups were determined a long time ago
(Bethe 1929) and have been used extensively in labelling the energy levels of molecules
(reviews and treatises include those of Eyring, Walter, and Kimball (1944), Nussbaum
(1968), Rosenthal and Murphy (1936), Slater (1963), and Wilson, Decius, and Cross
(1955)) in labelling the energy levels of ions or molecules in a crystal (reviews and
discussions include those of Herzfeld and Meijer (1961), Hutchings (1964), Judd
(1963), and McClure (1959a, b)) and also in labelling excitons in a crystal (Overhauser
1956). A particularly useful summary of the important properties of the crystallo-
graphic point groups and their representations is given by Koster, Dimmock, Wheeler,
and Statz (1963).

The theory that underlies the determination of the irreducible representations of
a space group was studied by Seitz (1936b) and first applied to symmorphic space
groups by Bouckaert, Smoluchowski, and Wigner (1936), to non-symmorphic space
groups by Herring (1942), and to double space groups by Elliott (1954b). Subse-
quently, many authors have determined the irreducible representations of individual
space groups and, in doing so, have employed many different sets of notation. A
substantial review was written by Koster (1957) and there have recently been pub-
lished some sets of complete tables of the irreducible representations of all the 230
space groups (Faddeyev 1964, Kovalev 1965, Miller and Love 1967, Zak, Casher,
Glück and Gur 1969). The importance of the irreducible representations of the space
groups lies in the fact that, as a result of Wigner's theorem, they can be used in
labelling the energy levels of a particle or quasi-particle in a crystal; they can therefore
be used in labelling the electronic energy band structure and the phonon dispersion
curves in a crystalline solid (for reviews see Blount (1962), Jones (1960), Nussbaum
(1966), Slater (1965b, 1967) on electronic band structure, and Maradudin and Vosko
(1968), Warren (1968) on phonon dispersion curves). Similarly, the irreducible repre-
sentations of a space group can also be assigned to the magnon dispersion curves in a
magnetic crystal. However, there is an added complication because the black and
white Shubnikov space groups possess *corepresentations* rather than ordinary repre-
sentations (Dimmock and Wheeler 1962b, Karavaev, Kudryavtseva, and Chaldyshev
1962, Loudon 1968, Wigner 1959, 1960a, b).

It is doubtful whether all the effort that workers have expended on the determina-
tion of point-group and space-group irreducible representations would be considered
worth while if the only result was a scheme for labelling energy levels. However, the
irreducible representations also enable one to determine the exact way in which a wave
function ψ_i will transform under the various operations of the Schrödinger group of
a molecule or crystal. This often enables some simplifications to be made when an
unknown wave function is expanded in terms of a set of known functions such as
spherical harmonics (Altmann 1957, Altmann and Bradley 1963b, Bell 1954, Betts

1959, McIntosh 1963, von der Lage and Bethe 1947) or plane waves (Cornwell 1969, Luehrmann 1968, Schlosser 1962, Slater 1965b, 1967). By restricting the expansion of an unknown ψ_i for an energy level E_i to those functions that are known to belong to the representation of E_i considerable simplifications can very often be achieved in the actual process of solving Schrödinger's equation to determine ψ_i. The knowledge of the transformation properties of the wave functions ψ_i is also of importance when considering a transition of a system between two energy levels E_i and E_j. It is then possible to use the condition that the quantum-mechanical matrix element of the transition is a pure number in order to determine, for any given perturbing potential, whether a given transition is allowed or forbidden, that is, to determine *selection rules*. The group-theoretical determination of selection rules for transitions in isolated molecules and in ions or molecules in crystals involves the study of products of various point-group representations and this is discussed in the references we have already mentioned. To use the knowledge of the transformation properties of ψ_i to study selection rules for transitions involving non-localized states in crystals is more complicated and initial work has been done by several authors (Birman 1962b, 1963, Elliott and Loudon 1960, Lax and Hopfield 1961, Zak 1962).

1.2. Group theory

We begin the mathematical work of this book by giving a short account of the theory of groups and their representations. We do not give proofs of theorems as these appear in the first few chapters of many well-known books such as those by Hamermesh (1962), Lomont (1959), Lyubarskii (1960), and Wigner (1959). For the sake of clarity, however, we illustrate some of the definitions and theorems by means of an example; for this purpose we use a group containing six elements which, as an abstract group we call G_6^2 (see Table 5.1) and which, in one of its realizations, is the symmetry group of an equilateral triangle.

There are two good reasons for starting with a preliminary account such as this. The first is that it makes clear what the background to the work is, and hence what it is recommended that the reader should be familiar with before proceeding with the rest of the book. The second reason is that it serves to introduce a large amount of notation; furthermore, when this is done on topics that are relatively familiar, then a reader can adjust himself more easily to the style and notation of the authors than if he is plunged immediately into new work.

The following set of definitions and theorems forms, therefore, the group-theoretical background to the work of this book. In later chapters some of them will be used as building blocks for further theorems that are either more advanced or more directly related to the study of solids. The groups that occur in the theory of solids have quite a complicated structure and, if the theorems needed for dealing with them are established rigorously and in complete detail, the proofs of such theorems require some advanced algebraic methods not commonly met in introductory courses on

group theory. Some of these methods appear in Chapter 4 and they rest heavily for their appreciation on the material in this section and the next.

DEFINITION 1.2.1. *Group.* A *group* **G** is a set of elements together with a binary composition called a *product* such that

    (i) the product of any two elements in the group is defined and is a member of the group: if $A, B \in \mathbf{G}$ then $AB \in \mathbf{G}$,

   (ii) the product is associative: $A(BC) = (AB)C$ for all $A, B, C \in \mathbf{G}$,

  (iii) there exists a unique identity‡ E in the group: $EA = AE = A$ for all $A \in \mathbf{G}$, and

  (iv) every element has a unique inverse‡ element: given $A \in \mathbf{G}$ there exists a unique element A^{-1} such that $AA^{-1} = A^{-1}A = E$.

DEFINITION 1.2.2. *Order of a group.* The number of elements in a group, **G**, is called the *order* of the group.

In what follows we shall be dealing only with *groups of finite order*. The symbol $|\mathbf{G}|$ is often used to denote the order of **G**.

DEFINITION 1.2.3. *Order of an element.* The *order of an element* $A \in \mathbf{G}$ is the least positive integer s such that $A^s = E$.

From Definition 1.2.1 it follows that a group is completely defined by its multiplication table. In fact, it is sufficient to give a set of relations involving certain elements from which the whole multiplication table can be constructed. The elements P_1, $P_2, \ldots, P_m$ of a group **G** are called a set of *generators* (or sometimes *generating elements*) if every element of **G** is expressible as a finite product of powers (including negative powers) of $P_1, P_2, \ldots, P_m$. The set of relations $g_k(P_1, P_2, \ldots, P_m) = E$ ($k = 1, 2, \ldots, s$) satisfied by the generators, which are sufficient to determine the whole multiplication table of **G** are called the *defining relations* (or sometimes *generating relations*) of **G**. For a lengthy discussion of generators and generating relations see, for example, the book by Coxeter and Moser (1965).

Example 1.2.1. In Table 1.1 we give the multiplication table for the group $\mathbf{G}_6^2$ of order 6 whose generators are P and Q and whose defining relations are $P^3 = E$, $Q^2 = E$, and $QP = P^2Q$. P is of order 3 and Q is of order 2.

Sets of generators and defining relations are not by any means unique; in fact it is often more straightforward to take more generators than are strictly necessary. There is always, of course, a minimum number of generators without which one

‡ It is not necessary to postulate the uniqueness and two-sidedness of the identity and of the inverse elements; for the existence of a right identity ($AE = A$) and right inverses ($AA^{-1} = E$) together with axioms (i) and (ii) is sufficient to establish uniqueness and two-sidedness. However these properties are so fundamental that many authors include them in their definition.

TABLE 1.1

The multiplication table for the group G_6^2.

E	P	P^2	Q	PQ	P^2Q
P	P^2	E	PQ	P^2Q	Q
P^2	E	P	P^2Q	Q	PQ
Q	P^2Q	PQ	E	P^2	P
PQ	Q	P^2Q	P	E	P^2
P^2Q	PQ	Q	P^2	P	E

Notes to Table 1.1.

(i) The generating relations of this group are: $P^3 = E$; $Q^2 = E$; $QP = P^2Q$.

(ii) In order to obtain a product LM take the element in the row beginning with L and the column headed M. Thus, for example, $(PQ)(P^2Q) = P^2$.

cannot generate the group, but if one uses such a minimal set the defining relations can sometimes be extremely complicated and it is to avoid such complications that one often takes an over-determined set of generators. However in the simple example above we do have a minimal set.

A geometrical realization of the above group is the set of symmetry operations that carry an equilateral triangle, $\triangle ABC$, into itself. If the intersection of the medians of $\triangle ABC$ is denoted by O then the operation P may be thought of as the 120 *anti-clockwise* rotation about a line through O perpendicular to the plane ABC and Q may be thought of as the reflection in the line AO. Equally well we could have taken P to be a 120° *clockwise* rotation and Q to be the reflection in BO, or for that matter in CO. In each case we would obtain the same group but with its elements labelled differently. This is a simple example of the non-uniqueness of a set of generators. In this example all six of the above sets of generators lead to the same defining relations; as we shall see in the next few paragraphs this is no accident, but on the other hand it must not be thought that different sets of generators always lead to the same defining relations.

DEFINITION 1.2.4. *Homomorphism, isomorphism*. Given two groups **G** and **G'**, a mapping θ of **G** onto **G'** which preserves multiplication is called a *homomorphism*. Thus for a homomorphism θ it follows that, for all $G_1, G_2 \in \mathbf{G}$,

$$(\theta G_1)(\theta G_2) = \theta(G_1 G_2). \tag{1.2.1}$$

If in addition θ is a one-to-one mapping it is called an *isomorphism*: **G** and **G'** are then said to be *isomorphic*. If θ is an isomorphism and $\mathbf{G} = \mathbf{G'}$ then θ is called an *automorphism*.

Example 1.2.2. Let $\mathbf{G} = \mathbf{G}_6^2$ and $\mathbf{G'} = \mathbf{G}_2^1$, the cyclic group of order 2 composed of elements E and P' with $P'^2 = E$ (E being the identity) (see Table 5.1). Then if θ is defined so that $\theta E = E, \theta P = E, \theta P^2 = E, \theta Q = P', \theta(PQ) = P'$, and $\theta(P^2Q) = P'$, then θ is a homomorphism of $\mathbf{G}_6^2$ onto $\mathbf{G}_2^1$.